

IPC Revision WG – Definition Project	Project: D005
	Subclass: C40B
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Rapporteur Proposal	

Title - C40B

Combinatorial chemistry, libraries, e.g. chemical libraries

Definition statement

This subclass covers:

- Methods of making libraries, e.g. combinatorial synthesis
- *In silico* or virtual conception of libraries; *in silico* or virtual libraries
- Chemical or biological libraries and modifications thereof, i.e. chemically, biologically or physically modified
- Methods of screening libraries or subsets thereof for a desired activity or property, e.g. binding ability
- Methods specially adapted for identifying the exact nature, e.g. chemical structure of a particular library member
- Apparatus specially adapted for use in combinatorial chemistry or library technology to identify library members, to screen libraries or to synthesize libraries; integrated apparatus specially adapted for performing any combination of these three tasks.
- Tags or linkers specially adapted for use in combinatorial chemistry or library technology.
- Other process or products specially adapted for combinatorial chemistry or libraries

Relationship between large subject matter areas

- Individual library members are classified in the appropriate places elsewhere in the IPC, e.g. in Section C, according to established procedure (see paragraphs 100 and 101 of the Guide). Subject matter that has a wider utility and may also be used outside combinatorial chemistry, e.g. solid supports and linkers of general utility in solid phase synthesis, general reagents, is classified in the appropriate places elsewhere in the IPC, e.g. [Section C](#).
- Methods or apparatus covered by this subclass are also classified for their biological, chemical, physical or other features in the appropriate places in the IPC, if such features are of interest, e.g.
 - Biocides [A 01 N](#)
 - Preparations for medical, dental or toilet purposes [A 61 K](#)
 - Therapeutic activity of compounds [A 61 P](#)
 - Separation [B 01 D](#)
 - Chemical or physical processes, e.g. catalysis; Apparatus therefor [B 01 J](#)
 - Chemical or physical laboratory apparatus [B 01 L](#)
 - Shaped plastics [B 29](#)

- Inorganic, organic or organic macromolecular compounds; Methods of preparation or separation thereof [C 01](#), [C 07](#), [C 08](#)
- Biochemistry, microbiology, enzymology including microorganisms or enzymes, preparing them, using them to synthesize compounds or compositions; Measuring or testing processes involving microorganisms or enzymes; Mutation or genetic engineering [C 12](#)
- Metal alloys [C 22](#)
- Chemical or physical analysis [G 01 N](#)
- Physical measurements methods; Apparatus therefore [G 01 R](#), [G 01 T](#)
- Photomechanical methods [G 03 F](#)
- Electrical digital data processing [G 06 F](#)
- Data processing [G 06 K](#)
- Image data processing [G 06 T](#)
- Displaying; Advertising [G 09 F](#)

References relevant to classification in this subclass

This [subclass](#) does not cover:

Examples of places where the subject matter of this class is covered when specially adapted, used for a particular purpose, or incorporated in a larger system:

Places in relation to which this [subclass](#) is residual:

Informative references

Attention is drawn to the following places, which may be of interest for search:

Special rules of classification within this subclass

- In this subclass, at each level of indentation, in the absence of an indication to the contrary, classification is made in the first appropriate place.
- When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.
- Unless otherwise stated, *in silico* or virtual libraries are classified in main-group C40B7/00 (or its subgroups) as if they were physically existing entities.

Glossary of terms

In this [subclass](#), the following terms or expressions are used with the meaning indicated:

Array:	Set of compounds maintained in a specified spatial distribution e.g. in the wells of a 96-well plate, in pins held in a rack or at the tip of optical fibers arranged in a bunch.
Biochemical method:	Process involving the use of <i>microorganisms</i> , enzymes, vectors or antibodies.
Chemical Evolution Process:	Process using <i>in vitro</i> selection systems that evolve to enrich mixtures of chemical compounds in those components having

selected properties. The terminology “directed molecular evolution” is commonly employed when the process is applied to mixtures of macromolecules (e.g. RNA aptamers). Selected compounds are then amplified (“copied”) using biochemical methods (e.g. enzymatic reverse transcription of RNA aptamers to DNA, PCR amplification and finally retranscription to RNA); This concept has been adapted to organic chemistry and opened a new branch of combinatorial chemistry named “dynamic combinatorial chemistry” wherein the enrichment in the (usually low-molecular weight) compounds having a selected property results from the equilibration process that carries out a preferential destruction and recycling of unselected compounds.

- Coding/encoding:** Strategy whereby a surrogate analyte is associated with each member of a library in order to record its structure and/or the reaction sequence used for its preparation. This is usually achieved by the use of tags/labels attached to the particles of solid support on which the library members are assembled.
- Combinatorial library:** A set of compounds (a library) prepared by combinatorial synthesis. May consist of a collection of pools or sub-libraries.
- Combinatorial synthesis:** Combinatorial synthesis is the preparation of sets of diverse entities by the combination of sets of chemical building blocks, e.g. reagents.
- Contained in:** A library contained in a microorganism, a cell or a vector is a library the members of which are present in the respective biochemical, e.g. in a plasmid.
- Decoding:** Method enabling the determination of the structure of a library member and/or the reaction sequence leading to its preparation, consisting in “reading” (e.g. determining the structure of) a surrogate analyte (code, tag, label) associated with said library-member.
- Deconvolution:** Process consisting of fractionating (normally by resynthesis, or by elaborating a partial library) a pool with some level of the desired activity to give a set of smaller pools. See also *iterative deconvolution*.
- Directed Molecular Evolution:** Directed Molecular Evolution is a process for enriching a library in members having a property or activity of interest. It involves cycles of taking a library, subjecting it to a screen to select for the desired property or activity, amplifying the “hits” to provide the starting library for the subsequent cycle.
“Mutations” may be introduced at the amplification stage in order to increase the diversity of the library. This subject matter involves aspects of creating and screening libraries.
- Displayed by:** A library displayed by a microorganism is a library present at the surface of such a microorganism, e.g. of a bacteria. See for example Nature Biotechnology (1997), 15, pages 29-34: “Display of heterologous proteins on the surface of microorganisms: from the screening of combinatorial libraries to live recombinant vaccines.
- Dynamic Library:** Collection of compounds (in solution) in dynamic equilibrium (i.e. constantly changing). If the composition of the library is altered by the presence of a target which selectively binds

certain library members, then shifting of the equilibrium will lead to an increase in the amount of those components which bind to the target with relatively high affinity. A dynamic library contains all the potentially possible combinations of the components undergoing dynamic random connection, whether these combinations are or are not actually present in the conditions used. It is a virtual library. A real entity is generated in the presence of the target.

- Fluorous Synthesis:** Approach for solution phase synthesis which takes advantage of the ability of highly fluorinated groups to partition out of aqueous and most organic solutions into a third phase consisting in a fluorinated solvent. The fluorinated side chain can act as a soluble support for synthesis.
- Identifying:** Determining the exact nature, e.g. chemical structure or sequence listing, of a particular library member or of a particular subset of library members.
- In silico* library:** A library which has no physical existence, being constructed solely in electronic form or on paper. It is one type of virtual library. The building blocks required for such a library may not exist, and the chemical steps for creating such a library may not have been tested. These libraries are used in the design and evaluation of possible libraries.
- "Integrated" apparatus:** Apparatus specifically designed for performing at least two different operations, e.g. synthesis and screening.
- Iterative deconvolution:** Method for the identification of active library members consisting in repeating the deconvolution strategy a certain number of times. Usually the initial library is divided into non-overlapping subsets. The subsets are tested (screened) separately, and the one with the greatest activity is identified. This subset is re-synthesized as a collection of simpler subsets which are tested for activity. The process is repeated until a unique library-member with (ideally) a high level of activity is identified.
- Library:** A library is a created collection of a plurality of compounds, microorganisms or other substances. The collection is useful as a test vehicle for determining which of its members or its subsets of members possess activities or properties of interest. A library might for example exist as:
- a solution
 - a physical admixture
 - an ordered or unordered array
 - a plurality of members present on a support and affixed thereto, e.g. by chemical bonding, by physical attractive forces or by coating.
- Liquid-phase synthesis:** In the context of C40B, this wording covers both solution phase syntheses (i.e. reactions involving only one liquid phase) as well as syntheses in multiple liquid phase systems (i.e. involving more than one liquid phase). The latter concern for instance syntheses performed on a liquid

macromolecular compound such as PEG (polyethylene glycol), on dendrimers, or wherein a fluorocarbon phase is present in the system (*fluorous synthesis*).

Microorganisms: bacteria, actinomycetales, fungi (e.g. yeast), virus, human, animal, or plant cells, tissues, protozoa or unicellular algae.

Particular attachment method: Specific method of attachment focusing on the way molecules are bound to the solid or liquid support, e.g. by means of electrostatic interactions, formation of covalent bonds by cycloaddition reactions or by irradiation.

Resin capture: Method consisting in contacting the reaction medium with a solid support after a reaction performed in solution, in order to attach the reaction product to the resin and thus collect it easily.

Safety-Catch Linker: A linker which is cleaved by performing two different reactions instead of only one, thus providing greater control over the timing of compound release. In practice, the resin is “activated” before the actual cleavage takes place (e.g. cleavage by nucleophilic displacement of a previously alkylated sulfonamide resin).

Screening: Determining whether a library contains a member or members which have a particular property or activity of interest.

Solid-phase synthesis: Synthetic process wherein the reactions are performed on a solid support, usually in the presence of a solvent, i.e. wherein one or more library building blocks are bound to a solid support (e.g. polymer, resin, glass beads) during library creation.

Solid support: Insoluble, functionalized, polymeric material to which library members or other reagents may be attached (often via a linker) allowing library members to be readily separated (by filtration, centrifugation, etc.) from excess reagents, soluble reaction by-products or solvents.

Solution-phase synthesis: Synthesis performed in solution, i.e. wherein the reactants and reagents are all soluble in the reaction medium (irrespective of the fact that, for instance, a supported catalyst is used during the reaction). It is also called “synthesis in solution”.

Traceless Linker: Linker which does not leave any residue on the cleaved compound, i.e. which is replaced by a hydrogen atom.

Virtual library: A library which has no physical existence. This terminology encompasses two different types of libraries: *in silico* libraries and dynamic libraries.

Synonyms and Keywords

In patent documents the following abbreviations are often used:

In patent documents the following expressions/words "----", "----" and "----" are often used as synonyms.

In patent documents the expression/word "----" is often used instead of "----" which is used in the classification scheme of this [subclass](#) (group).

In patent documents the expression/word "----" is often used with the meaning "----"